Can We Do Better with What We Have Done? Unveiling the Potential of ML Pipeline in Notebooks




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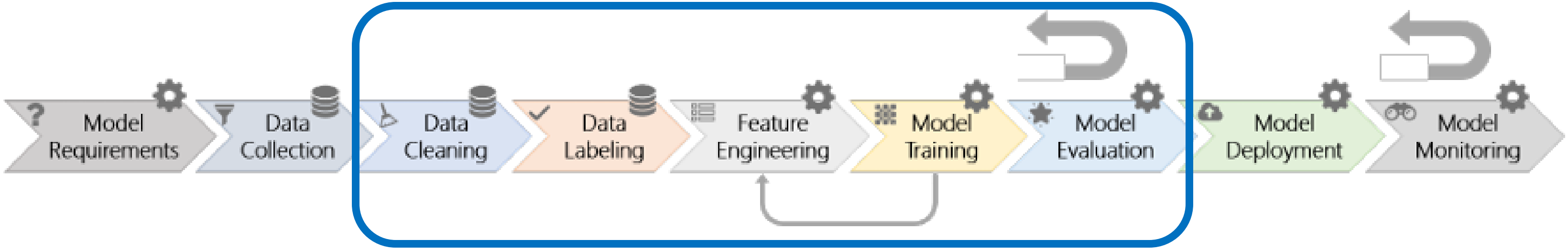
Exploratory Programming in Notebooks

To derive insights from a large amount of data by building high-performance ML model.



jupyterlab
colab
kaggle
nteract
Azure Notebooks
rmarkdown
RStudio

Exploratory Programming in Notebooks

- Linear structure
- Flexible
- Incremental

```
In [1]: import matplotlib.pyplot as plt
        from sklearn.cluster import KMeans
        from sklearn import datasets

In [2]: data = datasets.load_iris().data[:,2:4]
        petal_length, petal_width = data[:,0], data[:,1]

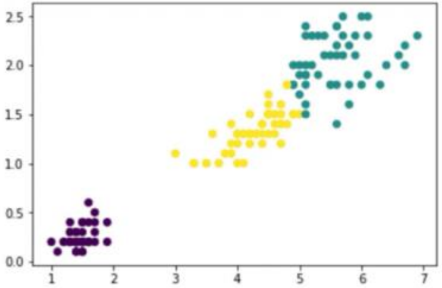
In [3]: print("Average petal length: %.3f" % (sum(petal_length) / len(petal_length),))

        Average petal length: 3.758

In [4]: clusters = KMeans(n_clusters=3).fit(data).labels_

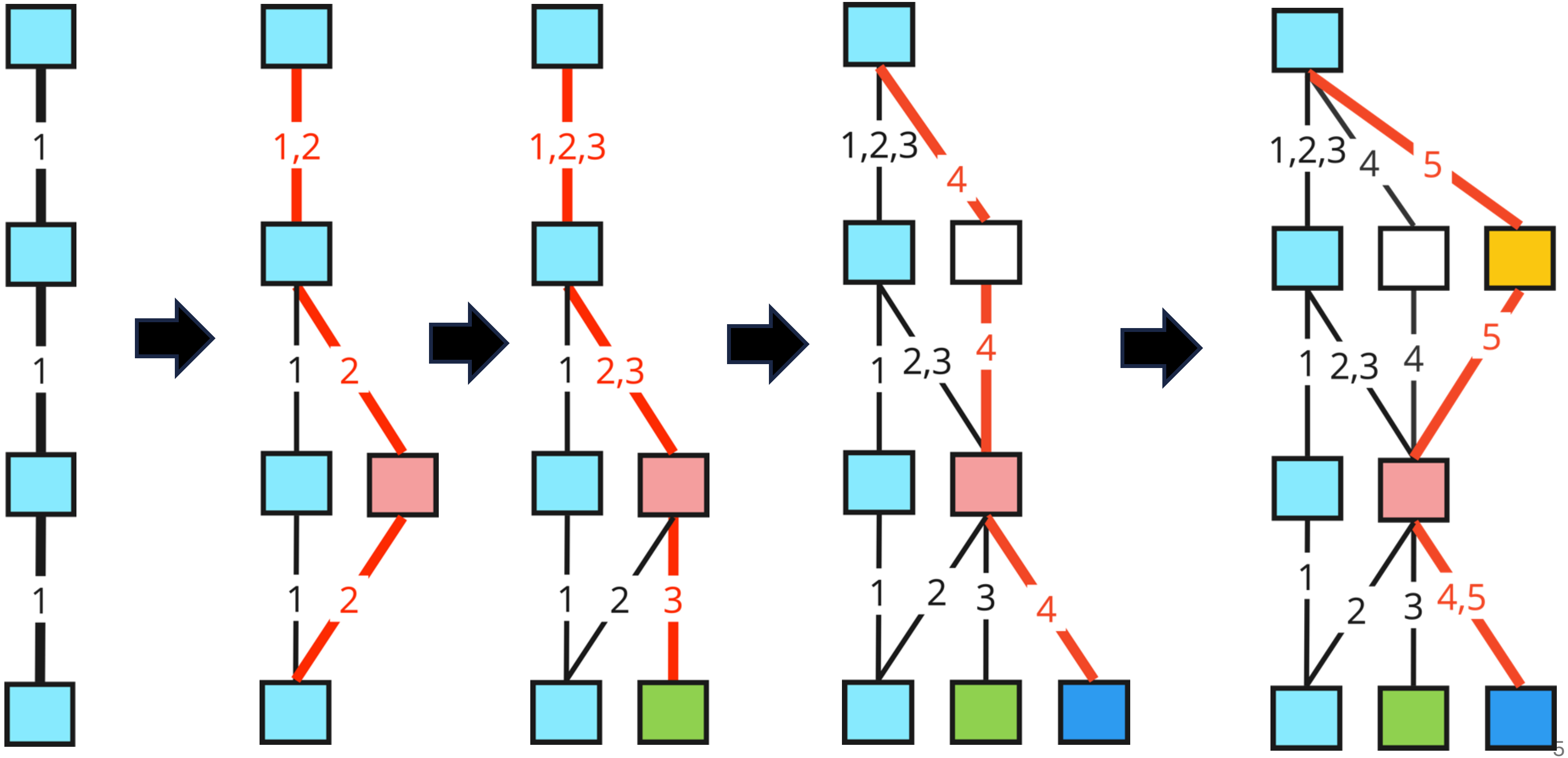
In [5]: plt.scatter(petal_length, petal_width, c=clusters)

Out[5]: <matplotlib.collections.PathCollection at 0x124e294e0>
```

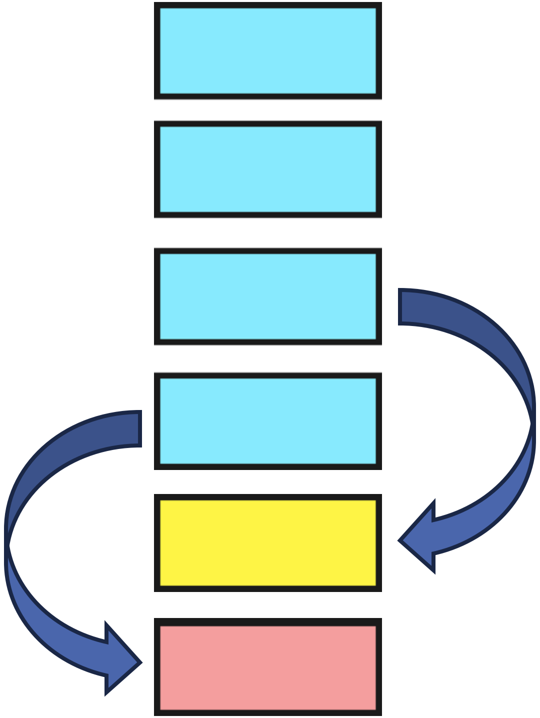



```
In [ ]: |
```

Evolution of ML Pipelines



Hard to Compare Alternatives Using Notebooks



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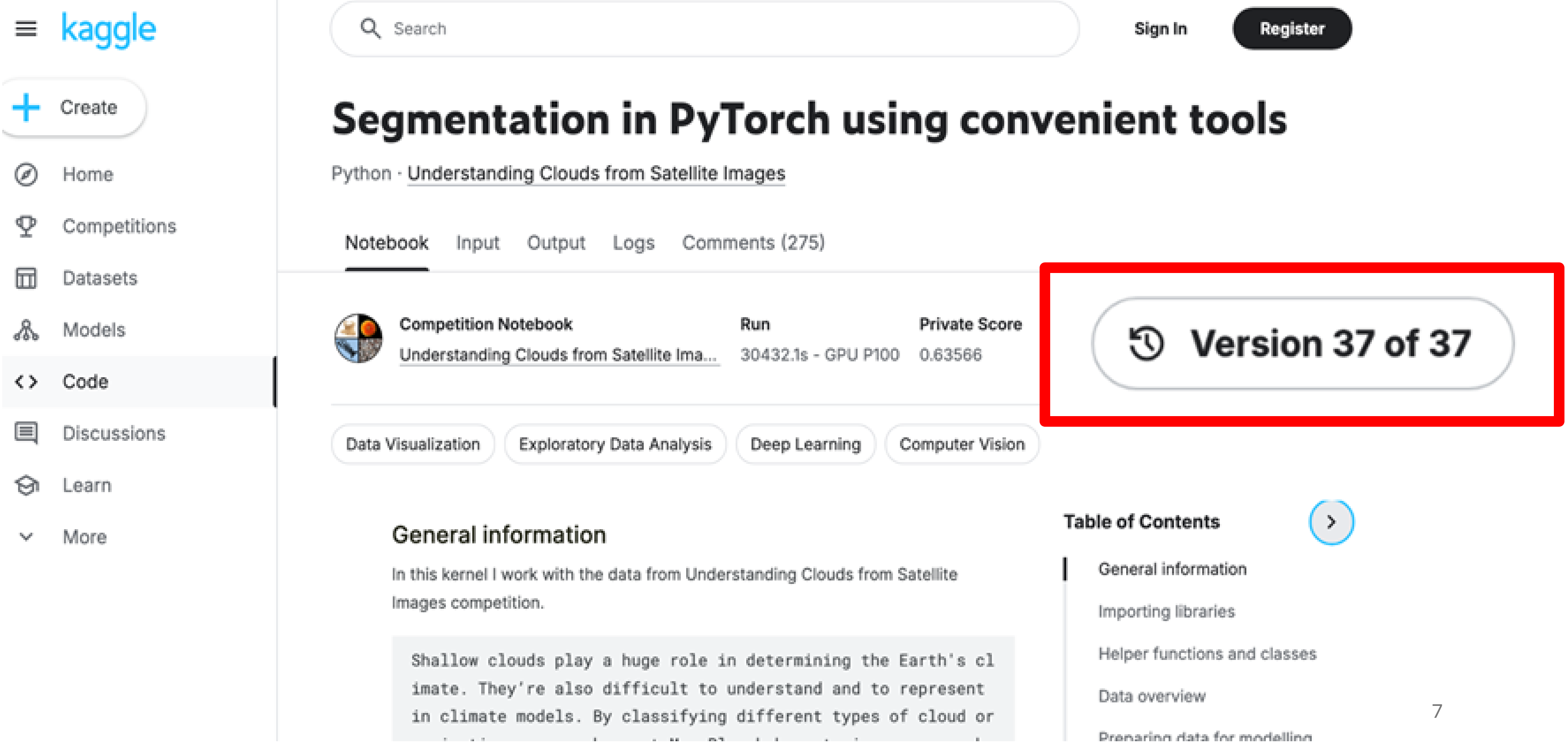

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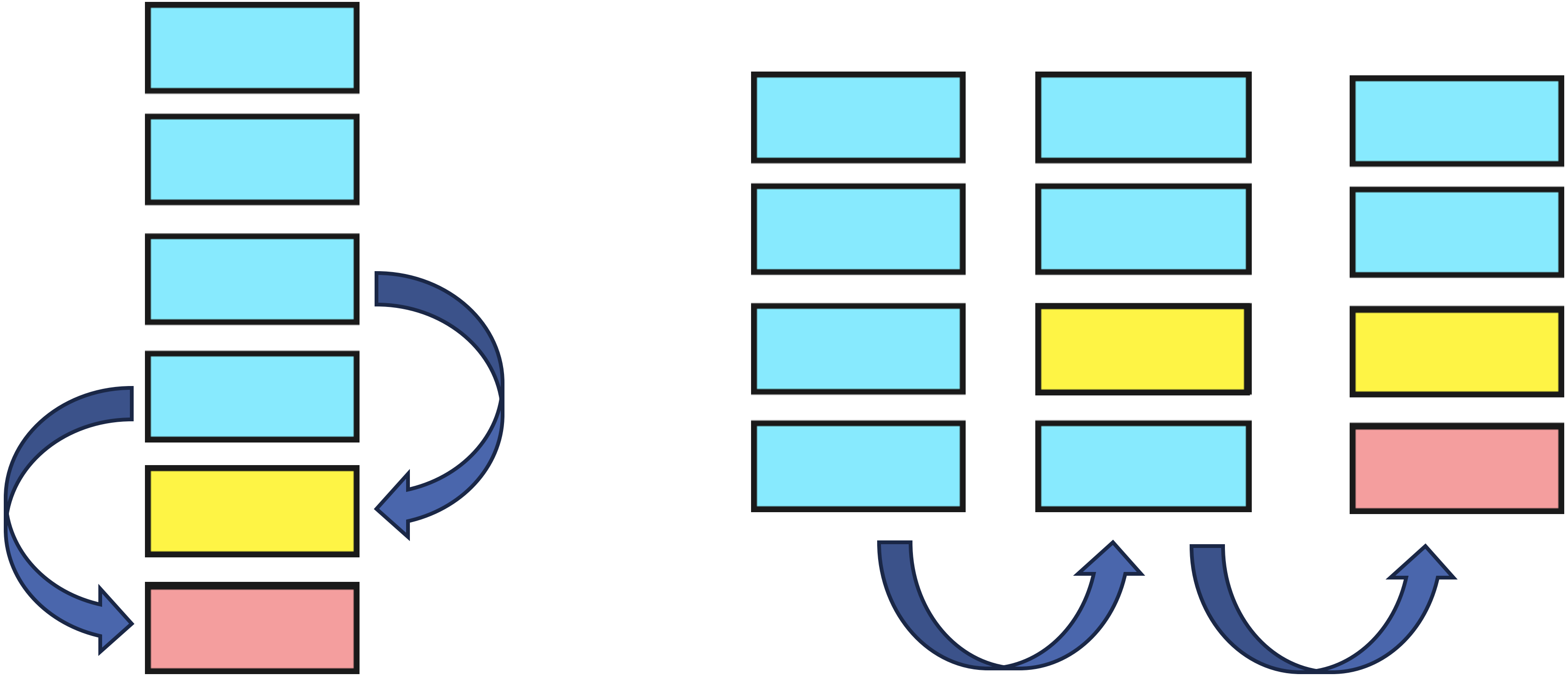

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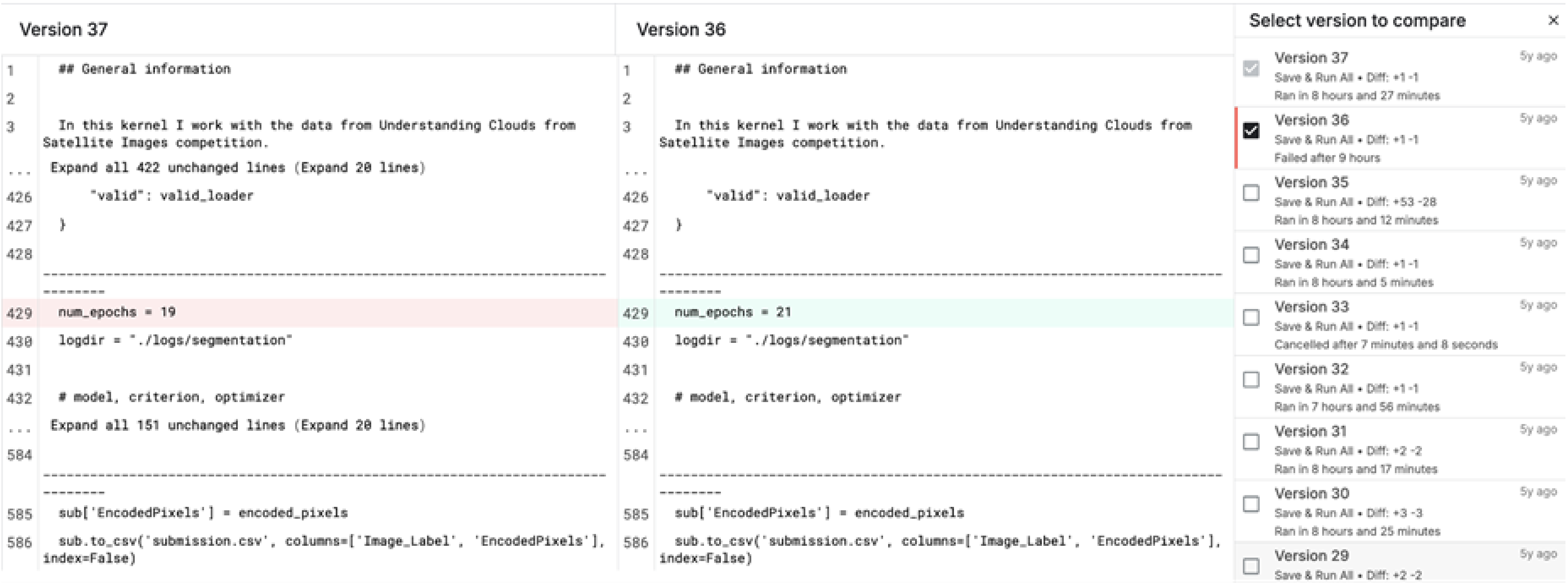
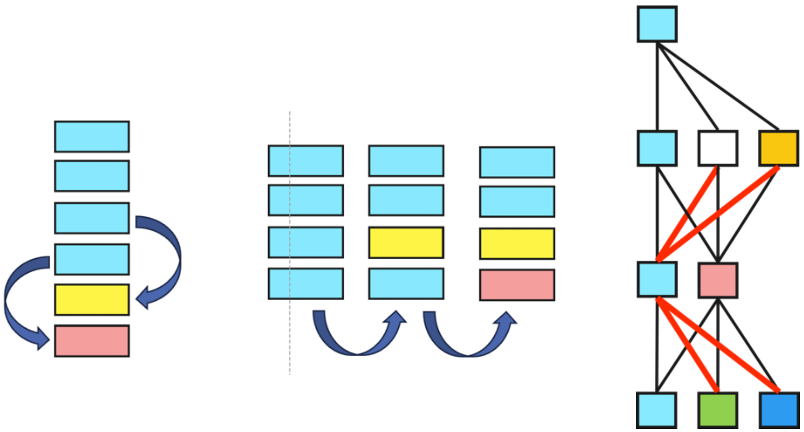


Observation



1x3x2x3 = 18 possible ML pipelines

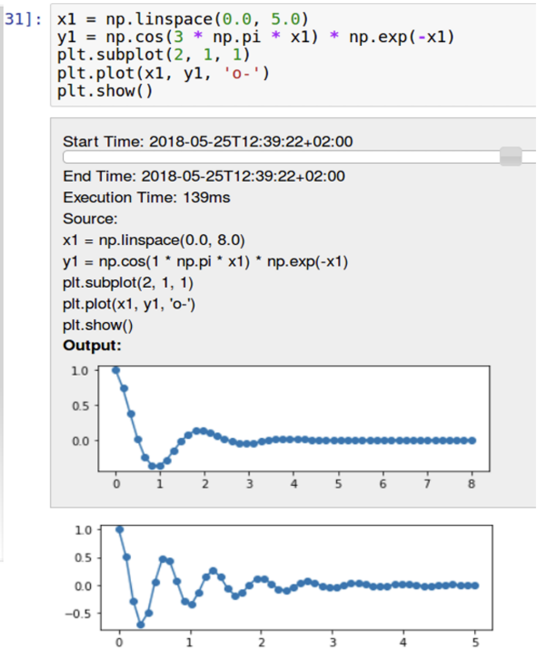
Search space can be huge

It might not be feasible to MANUALLY explore all the potential combinations

Prior Work on Supporting Exploration and Versioning in Notebooks

- Integrate a branching mechanism into the notebook [Weinman et al. 2021]

- Track the provenance of cells, enabling the comparison of successive cell versions [Samuel et al. 2018]



HOWEVER

While previous research focused on comparing alternatives for each cell, there is still a need to manually merge alternatives from various ML stages into a new pipeline, and then execute, document, and compare the outcomes.

Long-term Goal

To facilitate the automatic management and exploration of alternatives throughout the exploratory programming process, while preserving the inherent advantages of notebooks.

There remains a lack of systematic understanding of...

- How analysts explore the combination of alternatives across different ML stages?
- If these alternatives are comprehensively analyzed during the ML lifecycle?
- How to further support the exploration after extracting the diffs between versions of notebooks?

Research Questions

Current practices

Potential of unexplored ML pipelines

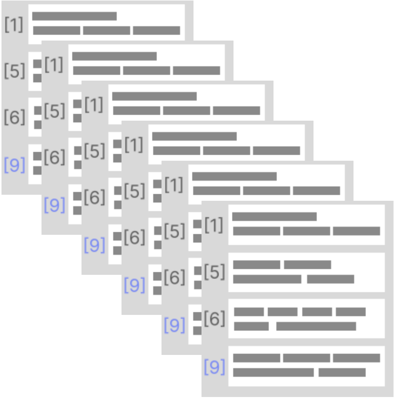
Research Questions

Current practices	RQ1: What are the alternatives? RQ2: How are alternatives explored?
Potential of unexplored ML pipelines	

Method - RQ1&2 (Current Practices)

MSR + Qualitative analysis

kaggle

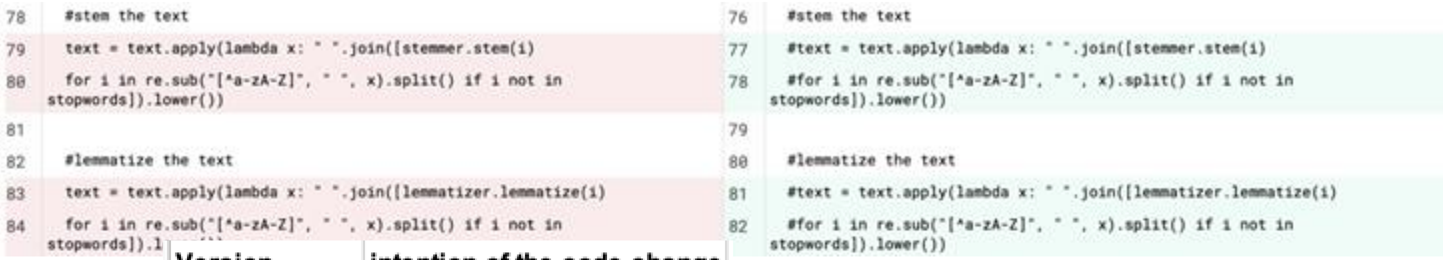


52 High-quality Python notebooks, 6 domains, minimum of 5 versions each, 930 versions of ML pipelines, 23385 LOC

Method - RQ1&2 (Current Practices)

Qualitative analysis

kaggle



```
78   #stem the text
79   text = text.apply(lambda x: " ".join([stemmer.stem(i)
80   for i in re.sub("[^a-zA-Z]", " ", x).split() if i not in
stopwords]).lower())
81
82   #lemmatize the text
83   text = text.apply(lambda x: " ".join([lemmatizer.lemmatize(i)
84   for i in re.sub("[^a-zA-Z]", " ", x).split() if i not in
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1	initial version
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4	failed
5	fix bug
6	create alternative, fix bug
7	no change
8	create alternative
9	failed
10	create alternative

Results - RQ1 (Types of Alternatives)

Data Preparation (DP)

data cleaning, preprocessing, and wrangling

Feature Engineering (FE)

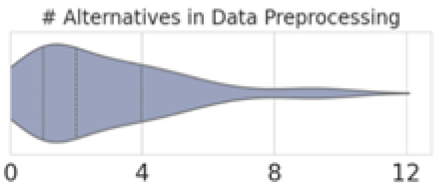
transforming raw data into relevant features

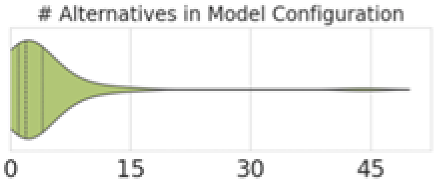
Model Configuration (MC)

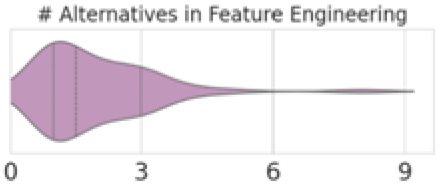
adjusting the parameters related to the architecture or individual components of the model

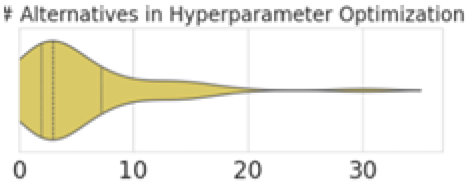
Hyperparam Optimization (HO)

adjusting various parameters that control the learning process



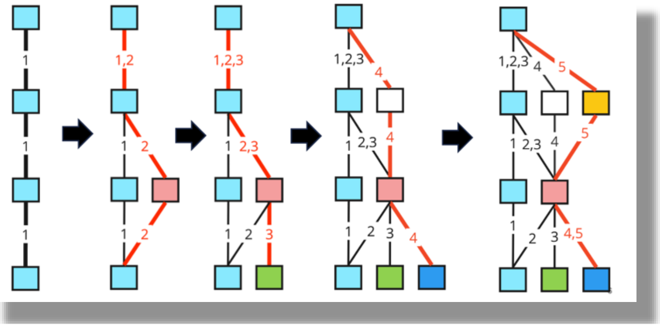




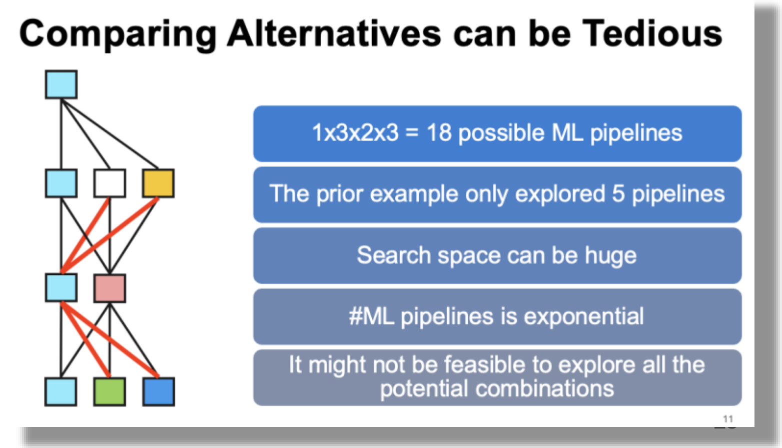


Results - RQ2
(How are alternatives explored?)

An iterative fashion



The median of our selected notebooks only represents 1.8% of all possible combinations.



Research Questions

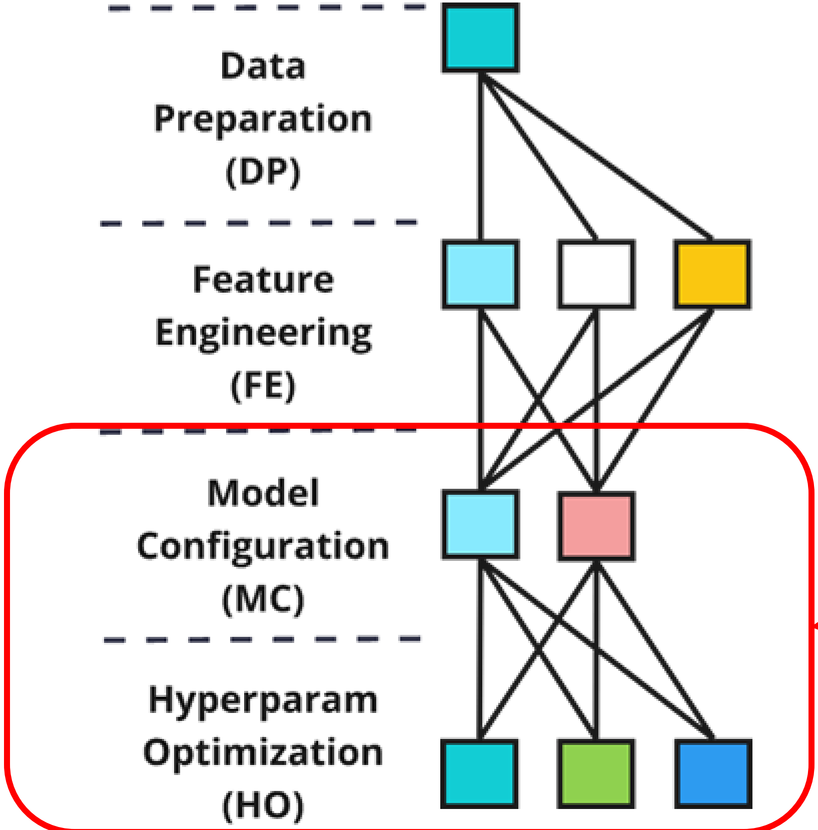
Current practices

RQ1: What are the alternatives?
RQ2: How are alternatives explored?

Potential of unexplored ML pipelines

RQ3: Evaluating unexplored ML pipeline
RQ4:
RQ5:

RQ4: Potential and capability of AutoML



replaced by

Research Questions

Current practices

RQ1: What are the alternatives?
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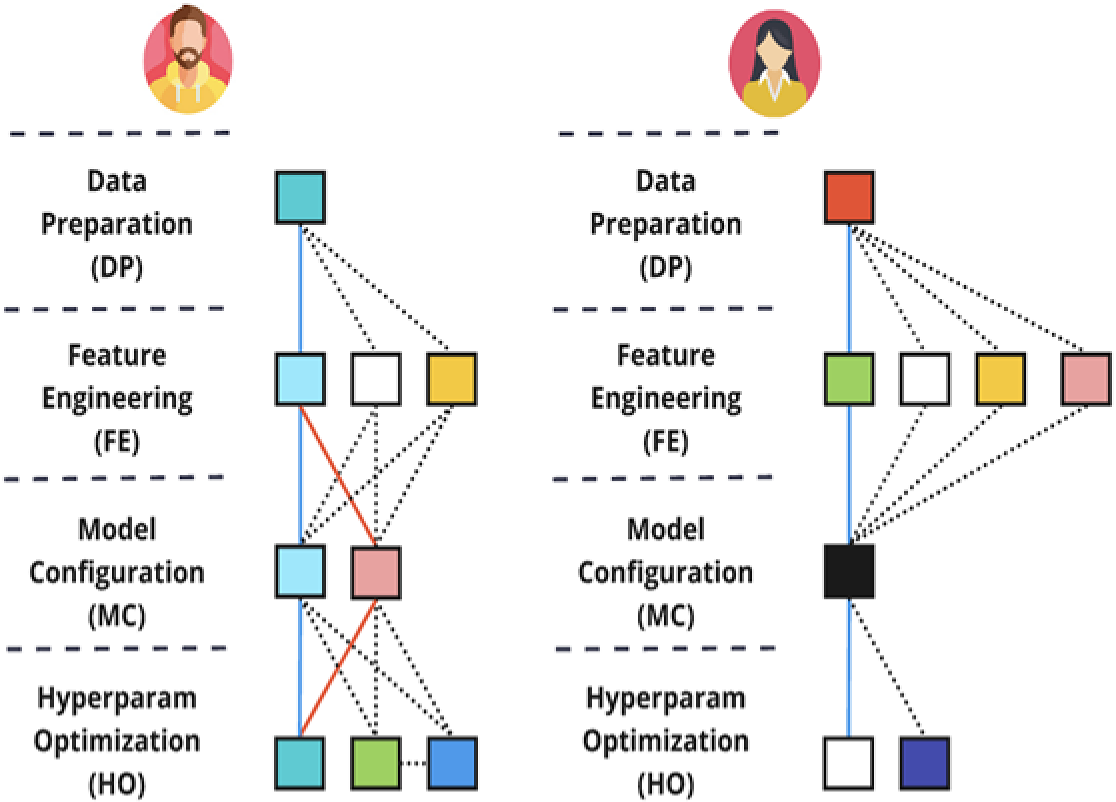
RQ3: Evaluating unexplored ML pipeline
RQ4: Potential and capability of AutoML

RQ5: Feasibility of Combining Alternatives from Different Analysts



RQ5: Will a combination of alternatives from different data scientists outperform the original notebook result? If yes, to what extent?

Research Questions

Current practices

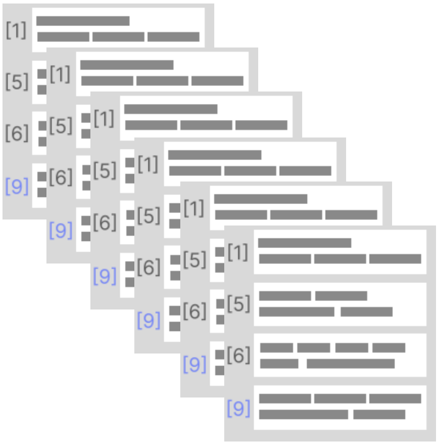
RQ1: What are the alternatives
RQ2: How are alternatives explored?

Potential of unexplored ML pipelines

RQ3: Evaluating unexplored ML pipeline
RQ4: Potential and capability of AutoML
RQ5: Crowdsourcing alternatives

Method to RQ3-5 (Unexplored ML Pipelines)

Ouantitative analysis



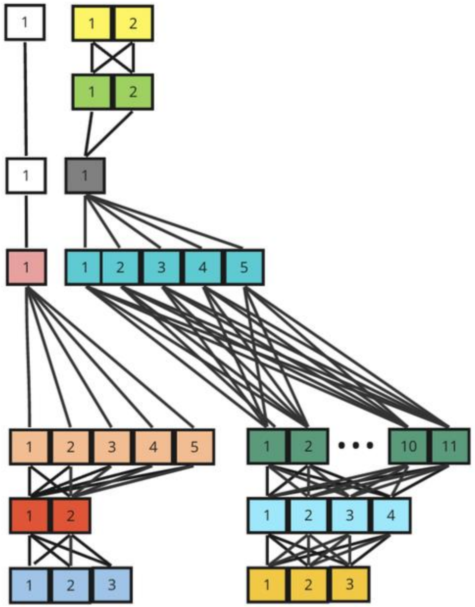
20 notebooks

11787 ML pipelines in total

Method - RQ3-5

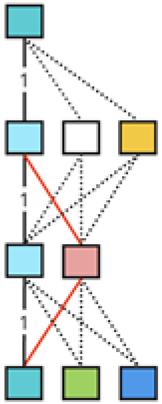
- If the search space is too big, we conduct experiments by randomly sampling a subset of pipelines.

NB5 has a total of 44,236,800 pipelines with a total approximated running time of 70,707,610 hrs



Results - RQ3
Potential of Unexplored Pipelines

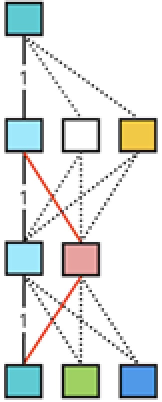
- 19/20 NBs contain unexplored pipelines



Results - RQ3
Potential of Unexplored Pipelines

- 19/20 NBs contain unexplored pipelines
- 16 NBs has performance increase

  (Avg 13.57%)
- 3 NBs have no performance increase



Results - RQ3
Potential of Unexplored Pipelines

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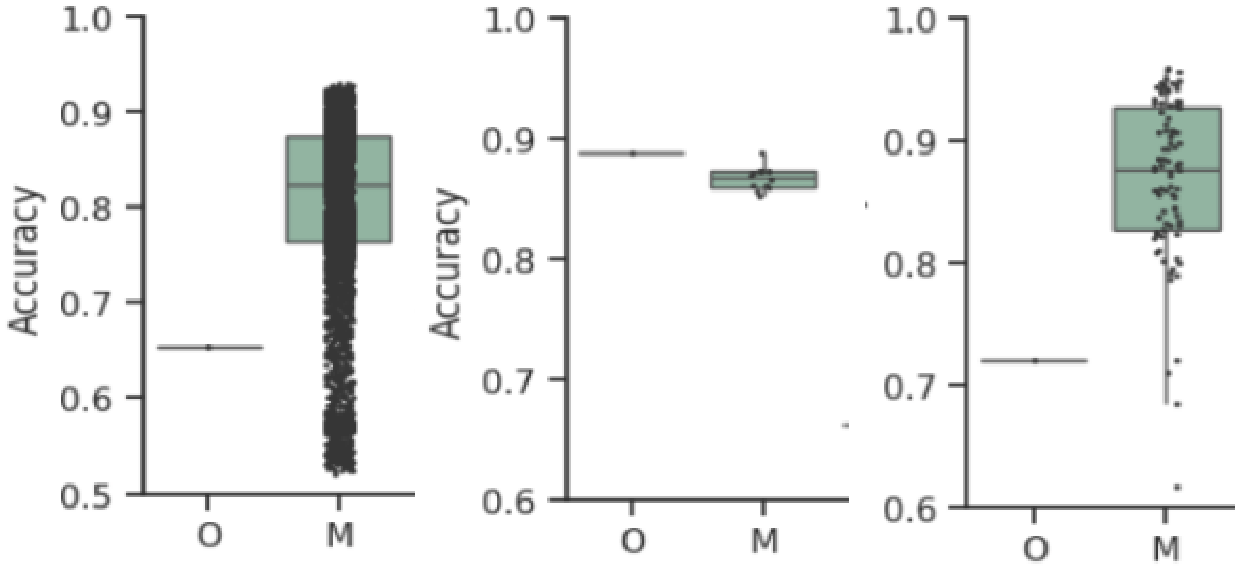

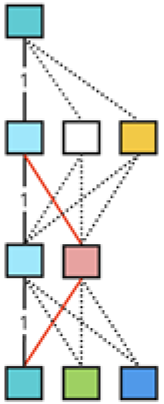

Research Questions

Current practices

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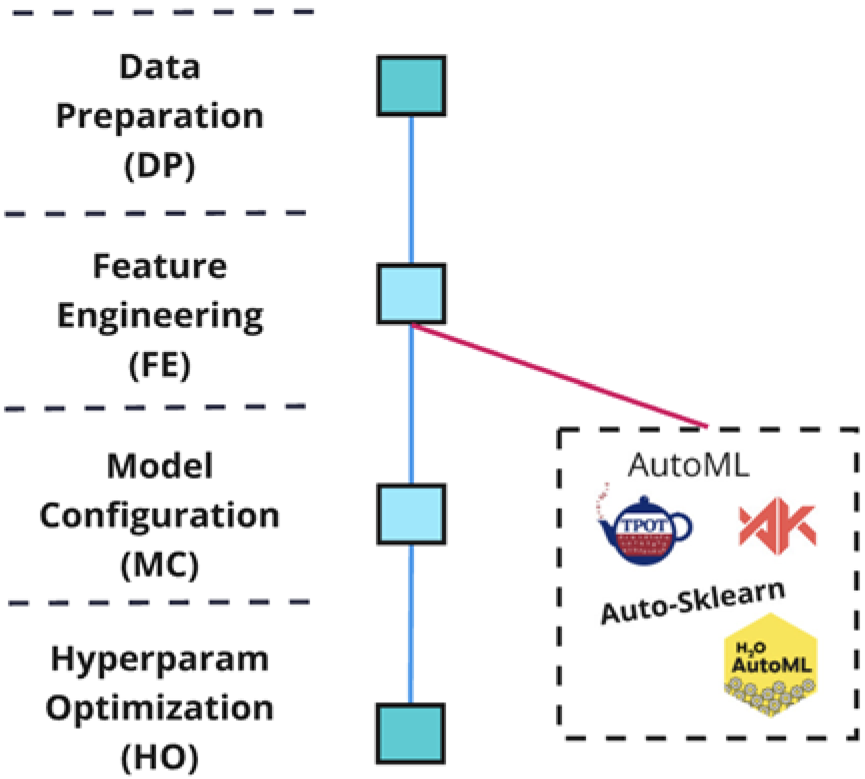
RQ2: How are alternatives explored?

Potential of unexplored ML pipelines

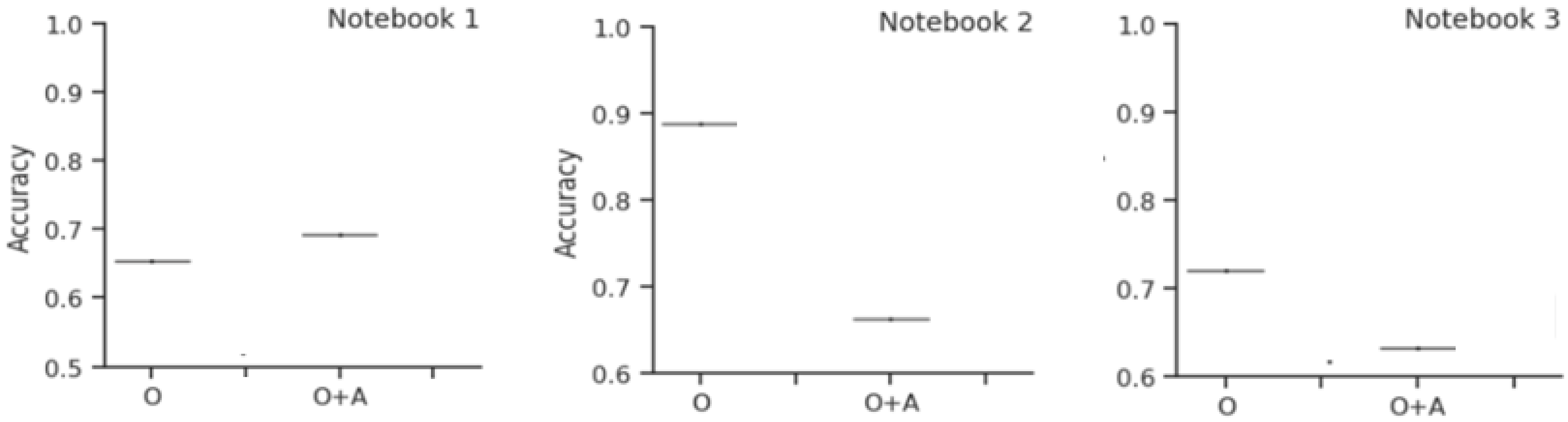
RQ3: Evaluating unexplored ML pipeline
RQ4: Potential and capability of AutoML
RQ5: Crowdsourcing alternatives

Results – RQ4
Evaluating AutoML in Exploratory Programming



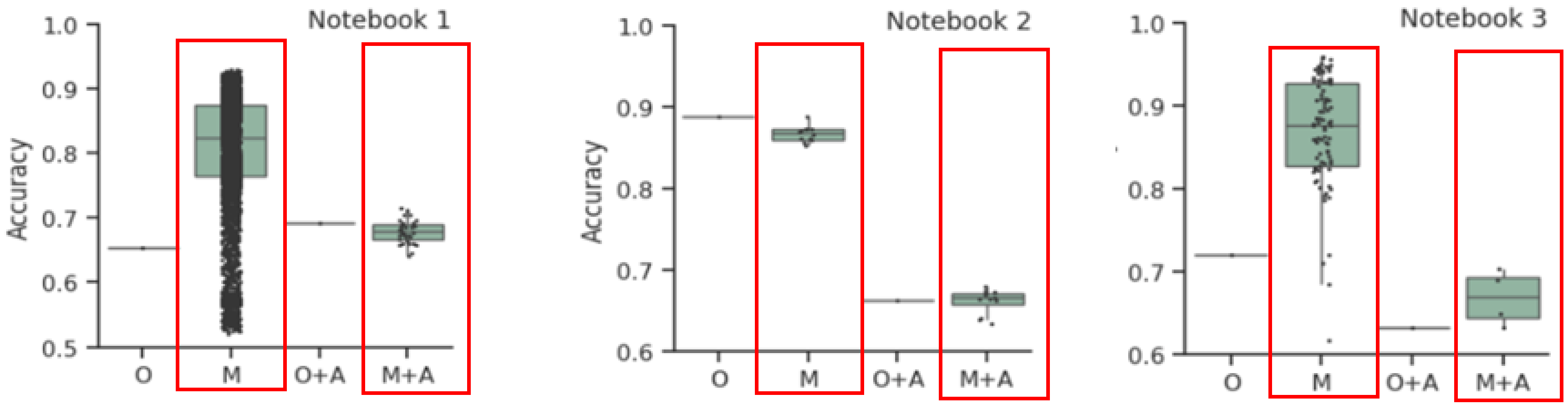
Results – RQ4
Original pipeline VS Original pipeline + AutoML

- 3/20 NBs show an average performance **increase** of 8.72%.
- 17/20 NBs show an average performance **decrease** of 16.59%.



Results of RQ4 (Cont.):
Merged pipeline VS Merged pipeline + AutoML

- 1/20 NBs have 8.14% performance increase due to a better set of hyperparameters
- 19/20 NBs have avg 17.41% performance decrease



Research Questions

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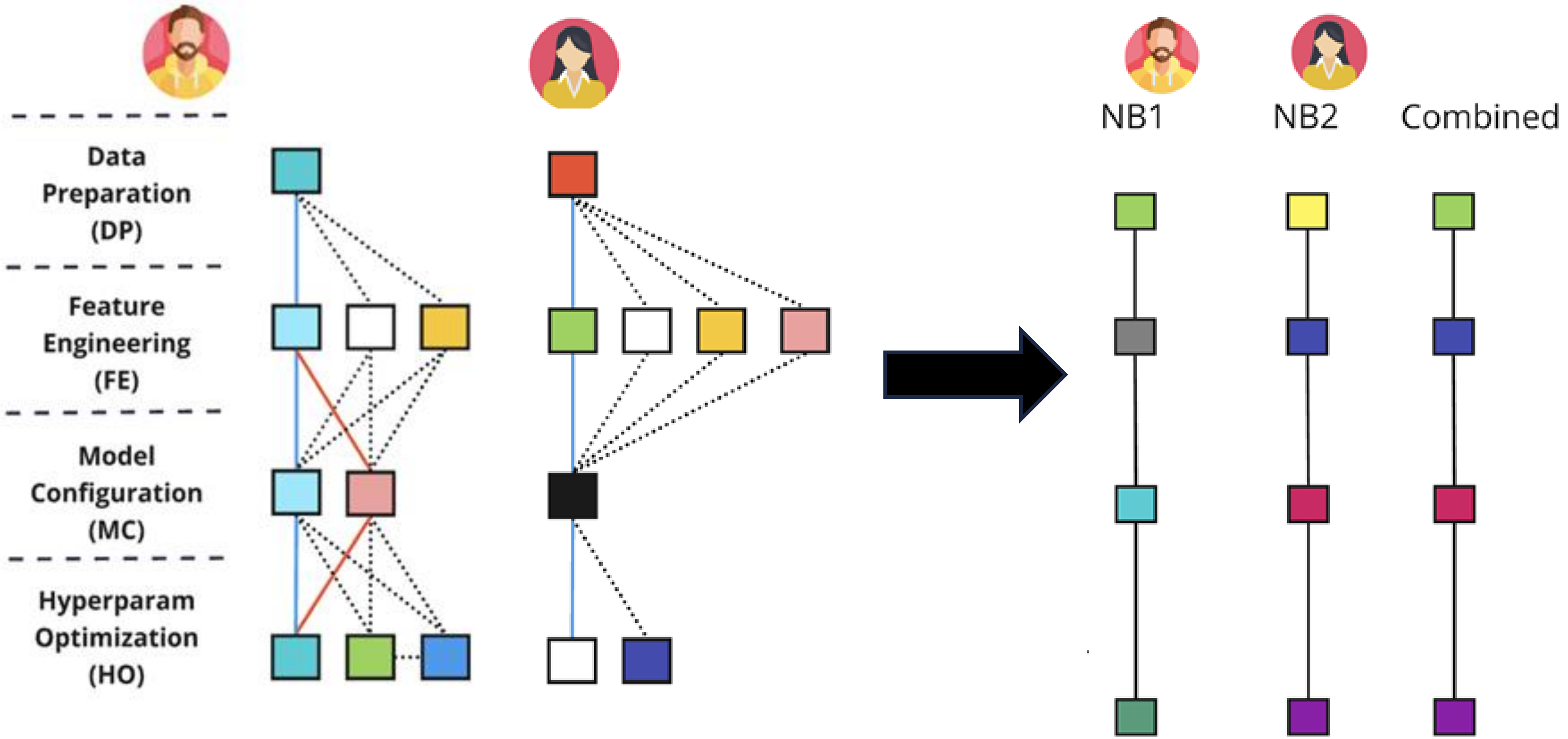
RQ5: Crowdsourcing Alternatives



Result - RQ5: Crowdsourcing Alternatives

3/10 NBs - avg 21.61%

4/10 NBs - avg 11.47%

3/10 NBs show operational errors

Finding: Despite the potential for improvement demonstrated in some notebooks, a **large amount of manual effort** is usually required to remove these inconsistencies for a successful integration.

Research Questions

RECAP

Current practices

RQ1: What are the alternatives
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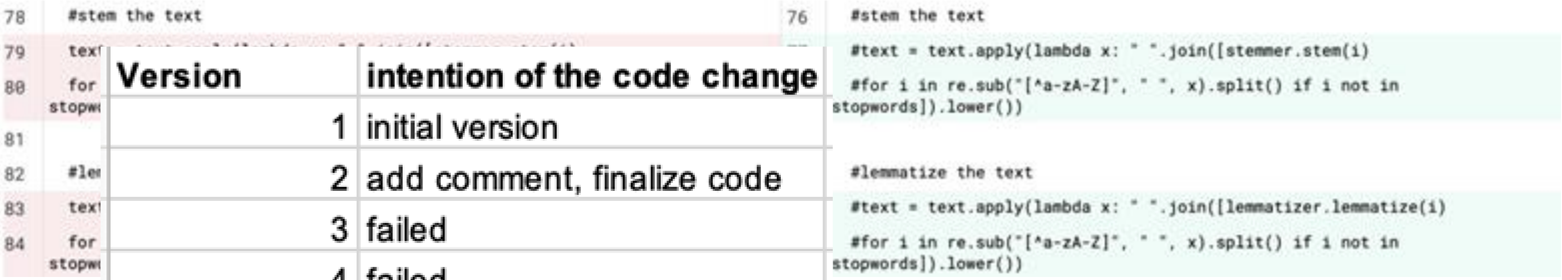
Tooling Opportunities & Research Directions

- More efficient ways to extracting and managing alternatives from large number of notebooks



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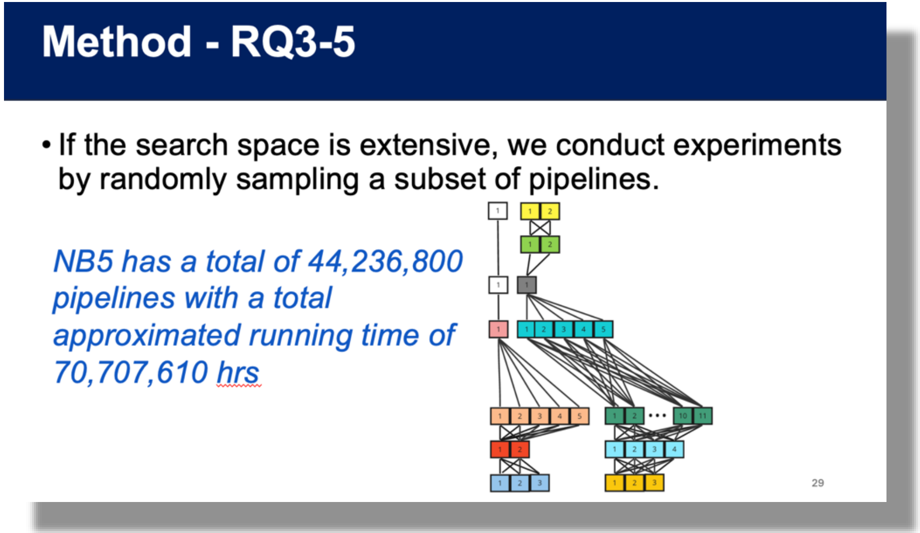
Tooling Opportunities & Research Directions

- More efficient ways to extracting and managing alternatives from large number of notebooks
- **More automated ways combine and execute merged pipelines is needed**

SPL?



Tooling Opportunities & Research Directions

- More efficient ways to extracting and managing alternatives from large number of notebooks
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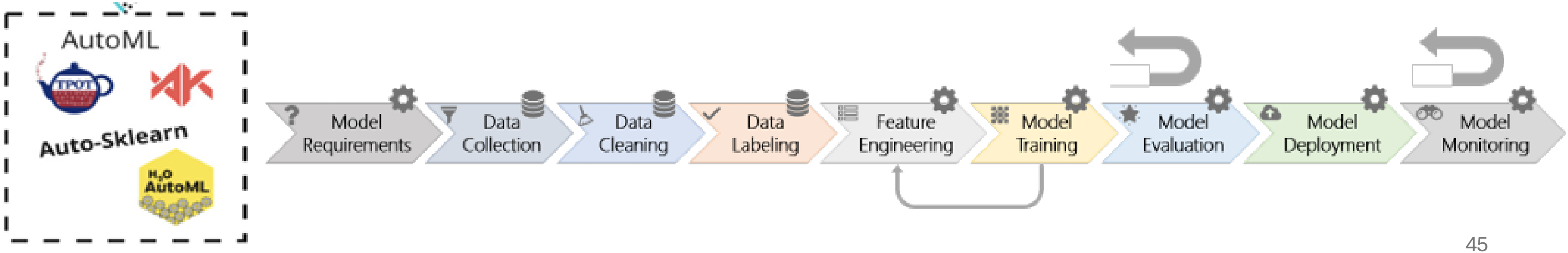
- **Better usability of AutoML tools during exploratory data analysis [Alamin et al. 2022]**



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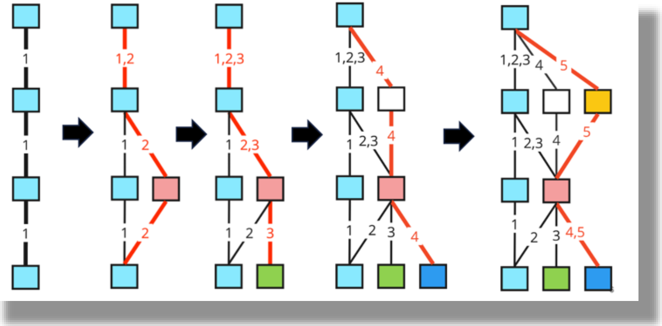

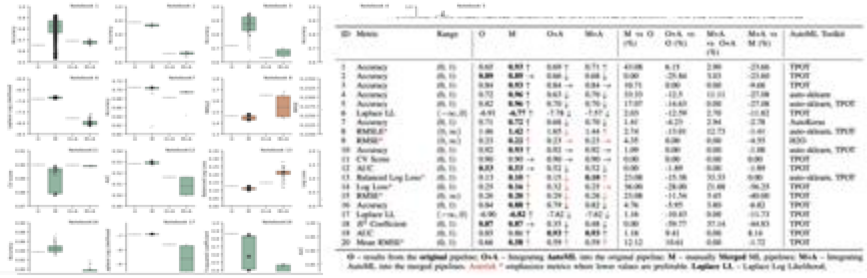

Research Questions

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- More efficient ways combine and execute merged pipelines is needed
- Better usability of AutoML tools during exploratory data analysis [Alamin et al. 2022]

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